Phases and phase transitions of quantum materials

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http://pantheon.yale.edu/~subir
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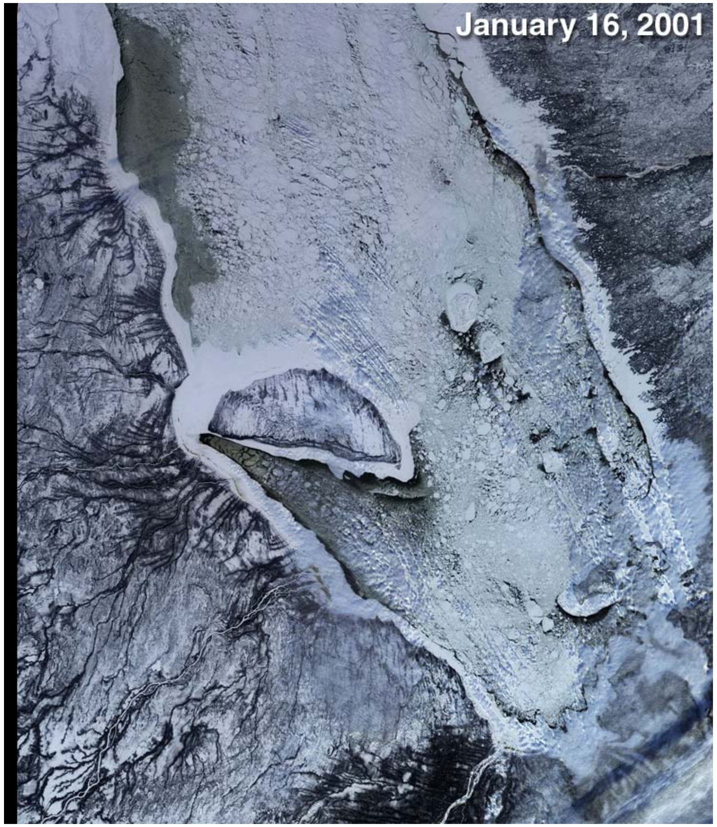
Phase changes in nature

Winter **James Bay** Summer



Ice

Water

At low temperatures, minimize energy

At high temperatures, maximize entropy

Classical physics: In equilibrium, at the absolute zero of temperature ($T = 0$), all particles will reside at rest at positions which minimize their total interaction energy. This defines a (usually) unique phase of matter *e.g.* ice.

Quantum physics: By Heisenberg's uncertainty principle, the precise specification of the particle positions implies that their velocities are uncertain, with a magnitude determined by Planck's constant $\hbar$. The kinetic energy of this $\hbar$-induced motion adds to the energy cost of the classically predicted phase of matter.

Tune $\hbar$: If we are able to vary the "effective" value of $\hbar$, then we can change the balance between the interaction and kinetic energies, and so change the preferred phase: matter undergoes a quantum phase transition

Outline

Varying "Planck's constant" in the laboratory

1. The quantum superposition principle – a qubit
2. Interacting qubits in the laboratory - $LiHoF_4$
3. Breaking up the Bose-Einstein condensate
   - Bose-Einstein condensates and superfluids
   - The Mott insulator
4. The cuprate superconductors
5. Conclusions

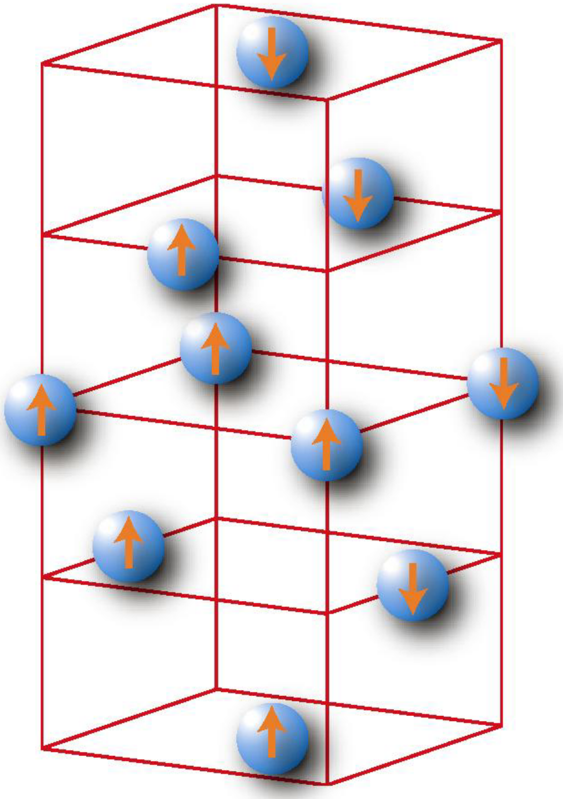
1. The Quantum Superposition Principle

The simplest quantum degree of freedom – a qubit

Two quantum states:

$$|\uparrow\rangle \text{ and } |\downarrow\rangle$$

These states represent *e.g.* the orientation of the electron spin on a Ho ion in $LiHoF_4$



Ho ions in a crystal of $LiHoF_4$

An electron with its "up-down" spin orientation uncertain has a definite "left-right" spin

$$|\rightarrow\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right)$$

$$|\leftarrow\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle - |\downarrow\rangle\right)$$

A $\rightarrow$ spin is a quantum superposition of $\uparrow$ and $\downarrow$ spins

2. Interacting qubits in the laboratory

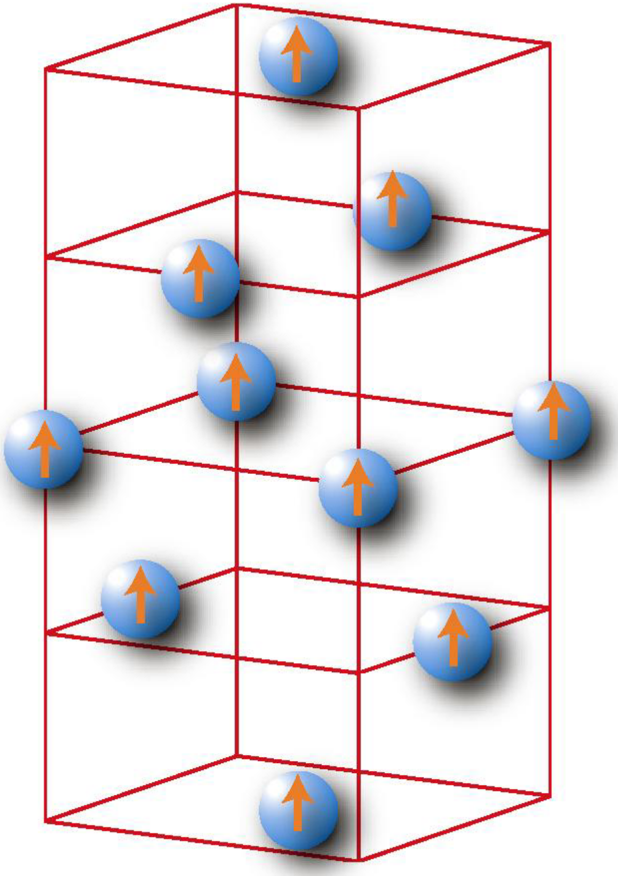
In its natural state, the potential energy of the qubits in $LiHoF_4$ is minimized by

$$|\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\ldots\ldots.\rangle$$

or

$$|\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\ldots\ldots.\rangle$$

A Ferromagnet



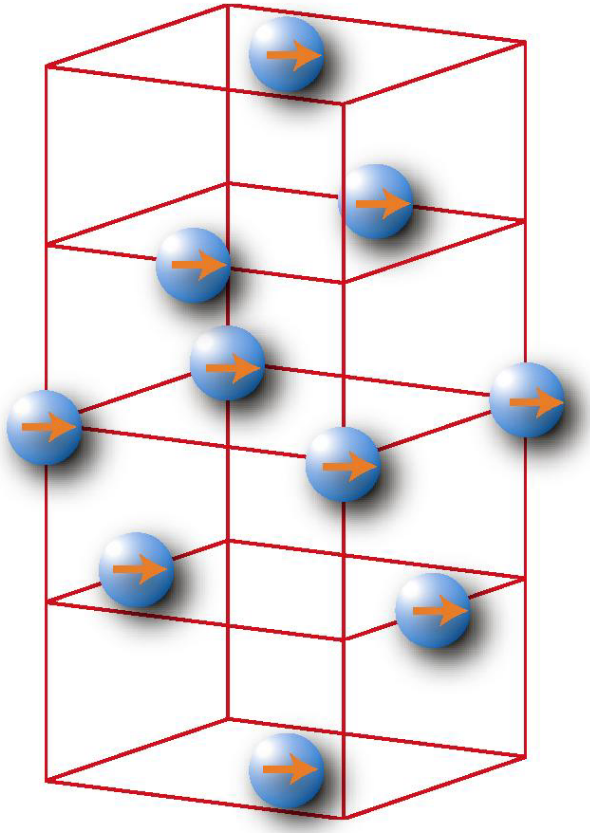
Enhance quantum effects by applying an external "transverse" magnetic field which prefers that each qubit point "right"

For a large enough field, each qubit will be in the state

$$|\rightarrow\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right)$$

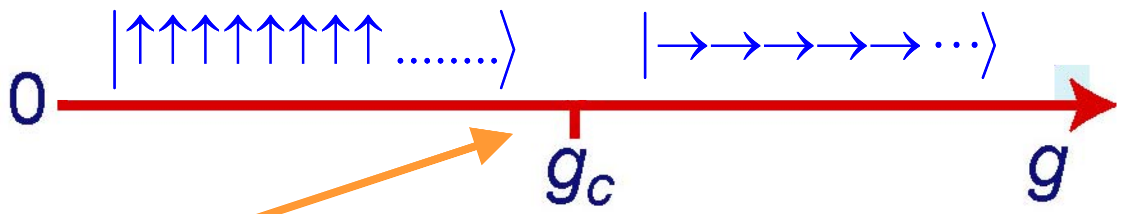
The qubits are collectively in the state

$$
\begin{aligned}
|\rightarrow\rightarrow\rightarrow\cdots\rangle = {} & |\uparrow\uparrow\uparrow\cdots\rangle + |\downarrow\uparrow\uparrow\cdots\rangle + |\uparrow\downarrow\uparrow\cdots\rangle \\
& + |\uparrow\uparrow\downarrow\cdots\rangle + |\downarrow\downarrow\uparrow\cdots\rangle + |\uparrow\downarrow\downarrow\cdots\rangle \\
& + |\downarrow\uparrow\downarrow\cdots\rangle + |\downarrow\downarrow\downarrow\cdots\rangle \\
\neq {} & |\uparrow\uparrow\uparrow\cdots\rangle + |\downarrow\downarrow\downarrow\cdots\rangle
\end{aligned}
$$



Phase diagram

Absolute zero of temperature



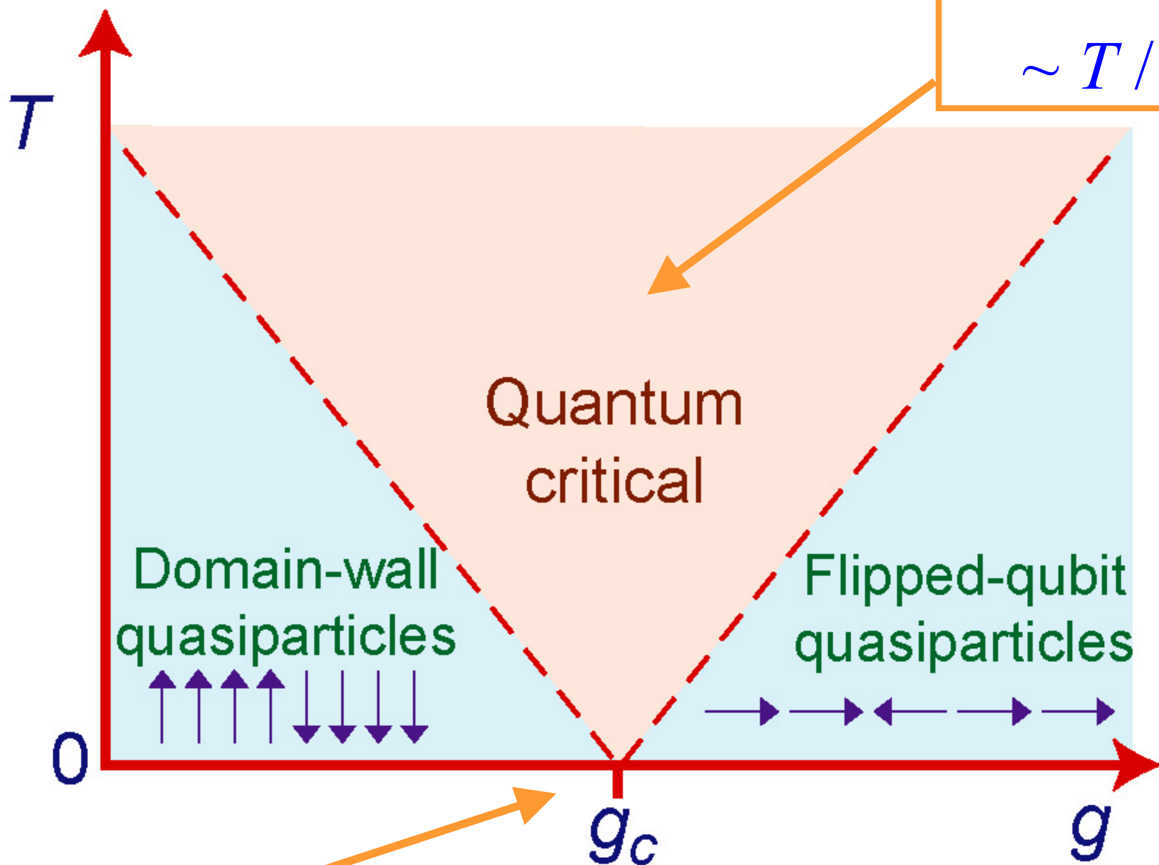
g = strength of transverse magnetic field

Quantum phase transition

Phase diagram

Spin relaxation rate

$\sim T / \hbar$



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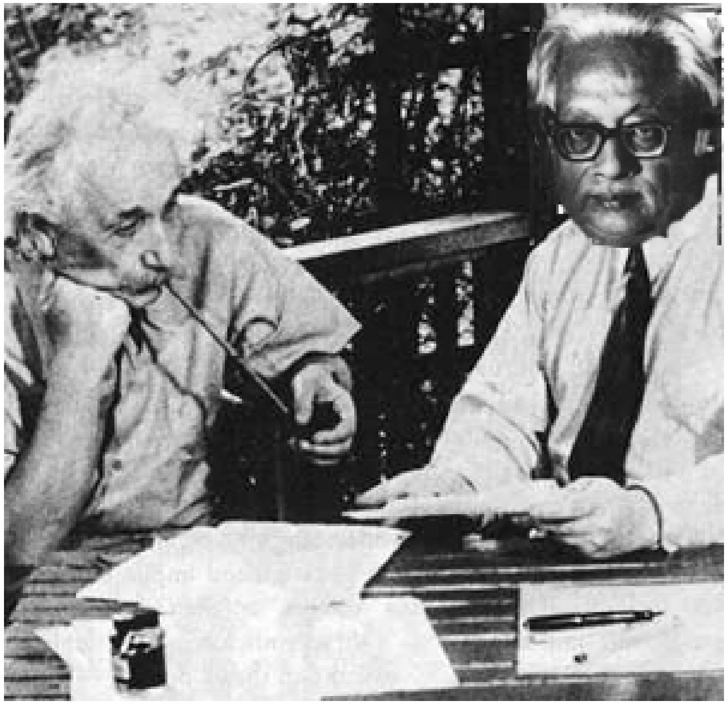
Quantum phase transition

3. Breaking up the Bose-Einstein condensate

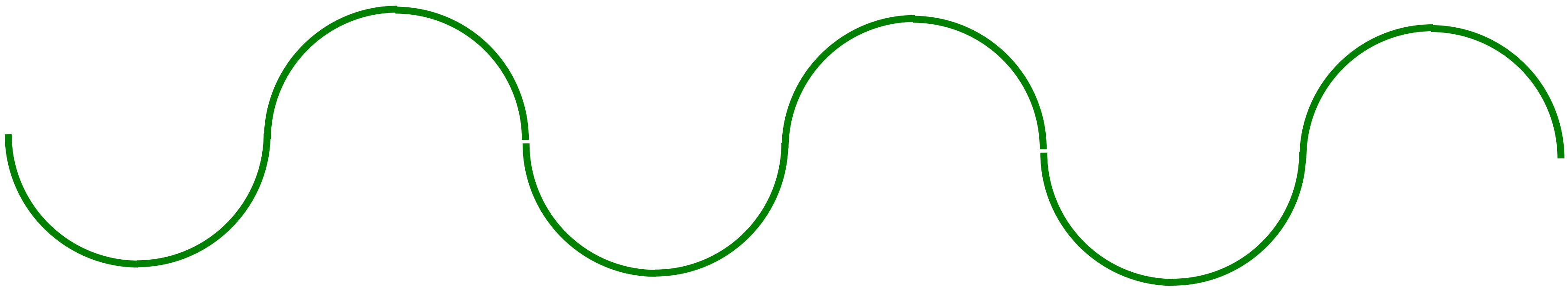
Certain atoms, called ***bosons*** (each such atom has an even total number of electrons+protons+neutrons), condense at low temperatures into the same single atom state. This state of matter is a Bose-Einstein condensate.



A. Einstein and S.N. Bose (1925)

The Bose-Einstein condensate in a periodic potential

"Eggs in an egg carton"



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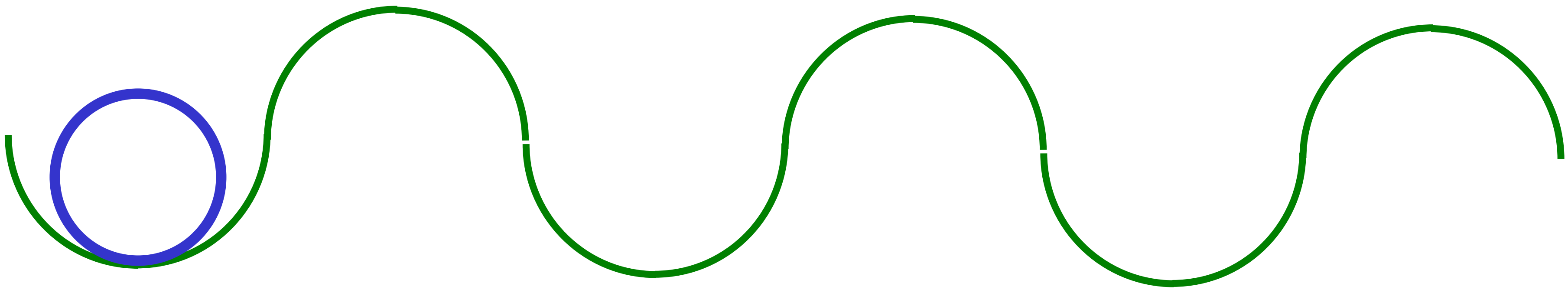

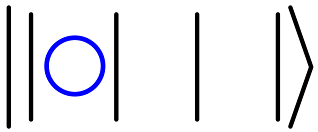

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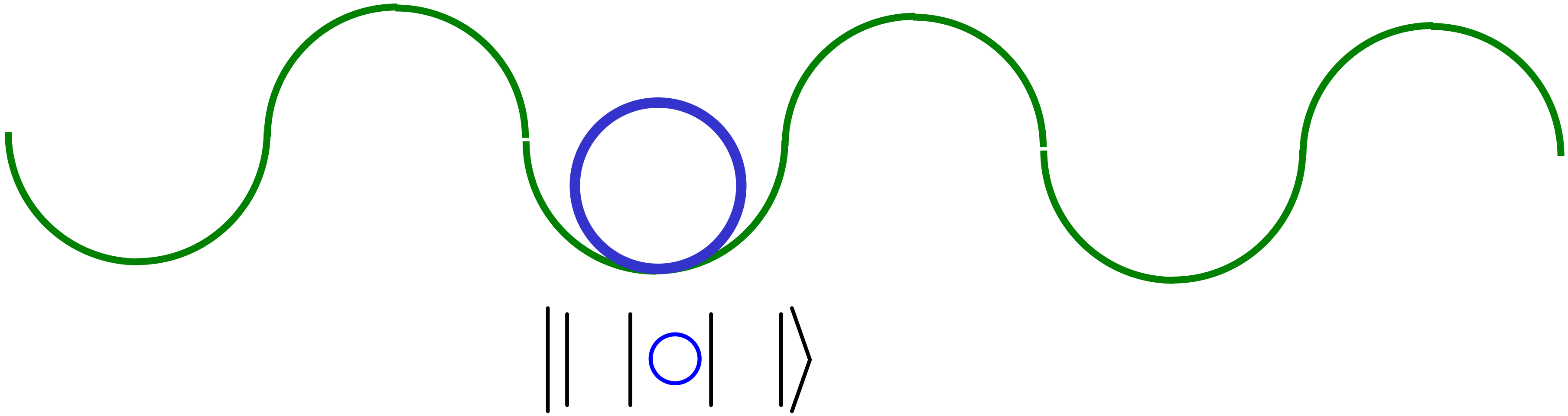

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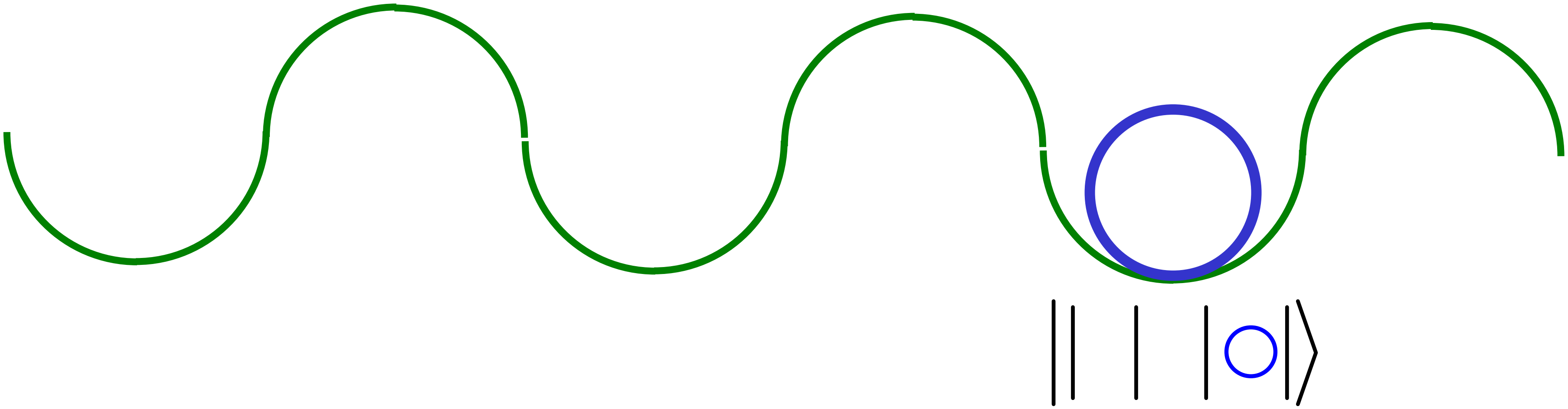

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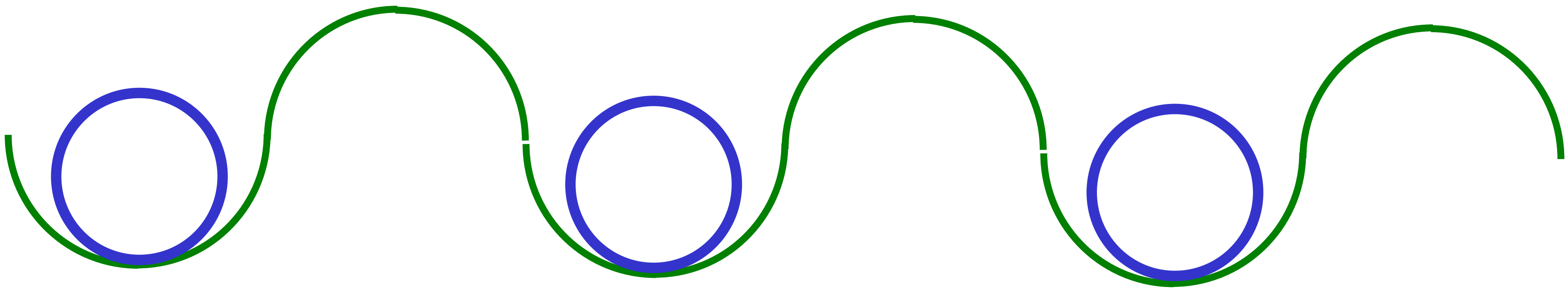
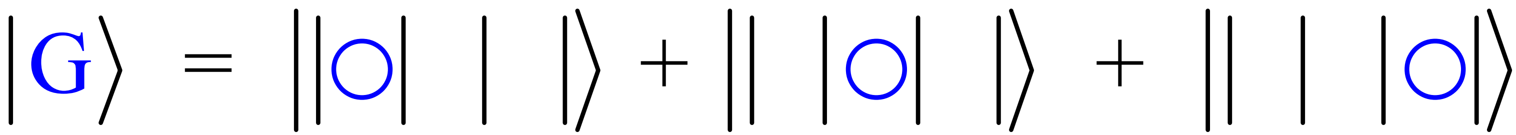


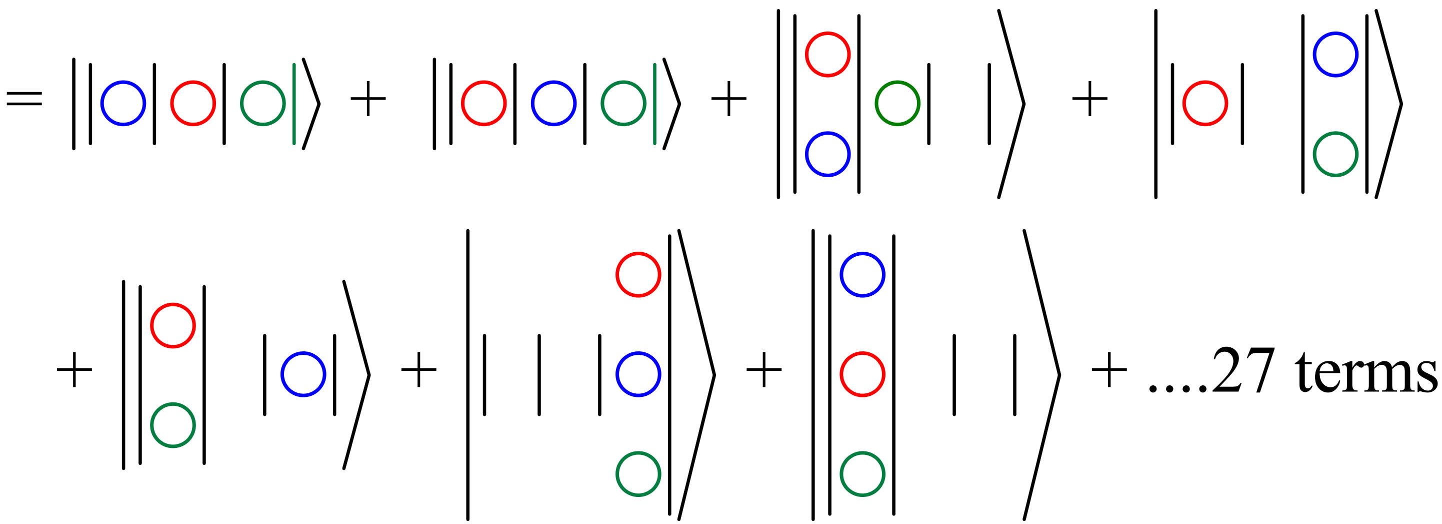


Lowest energy state of a single particle
minimizes kinetic energy by maximizing
the position uncertainty of the particle

The Bose-Einstein condensate in a periodic potential

Lowest energy state for many atoms

$$|\mathrm{BEC}\rangle = |\mathrm{G}\rangle|\mathrm{G}\rangle|\mathrm{G}\rangle$$



Large fluctuations in number of atoms in each potential well – *superfluidity* (atoms can "flow" without dissipation)

The Bose-Einstein condensate in a periodic potential

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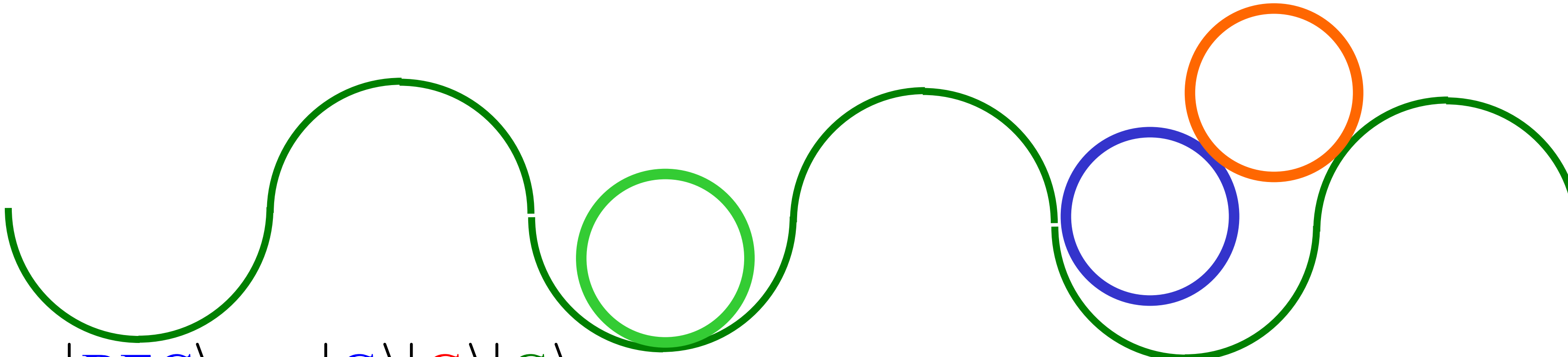
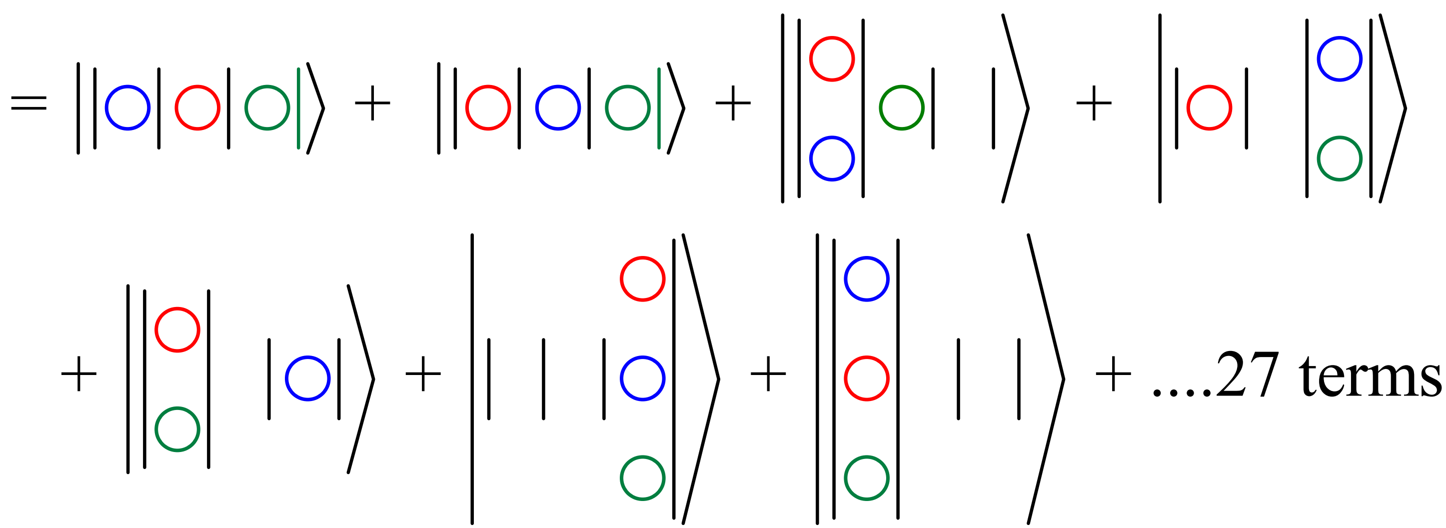


$$|\mathrm{BEC}\rangle = |G\rangle|G\rangle|G\rangle$$



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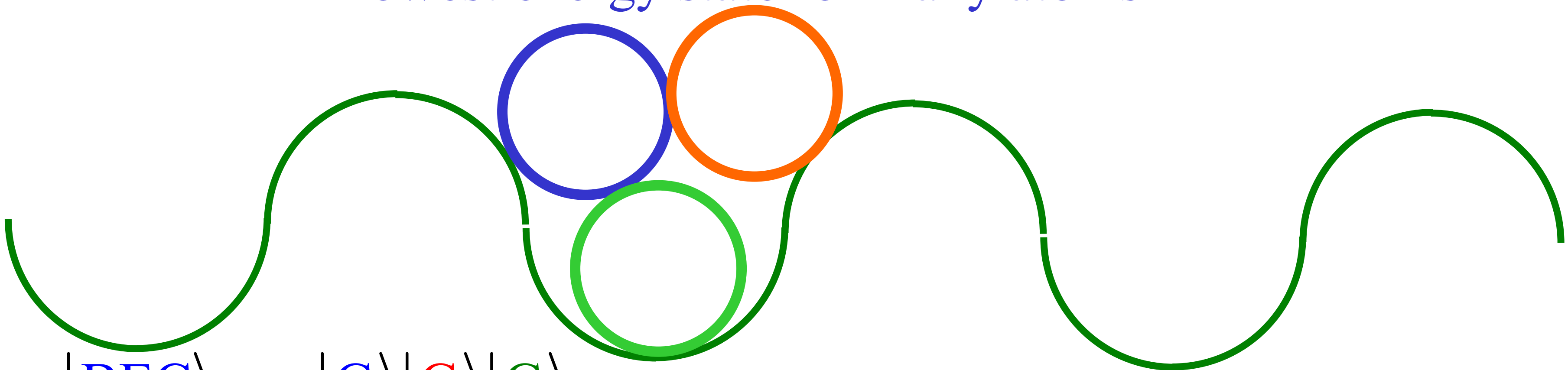

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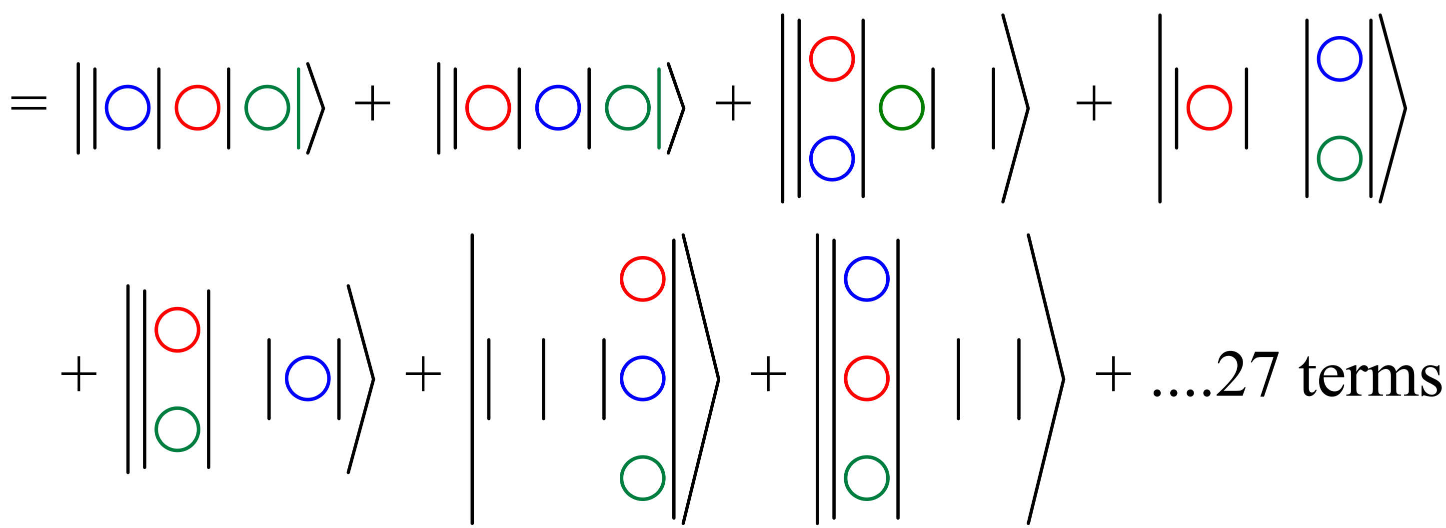

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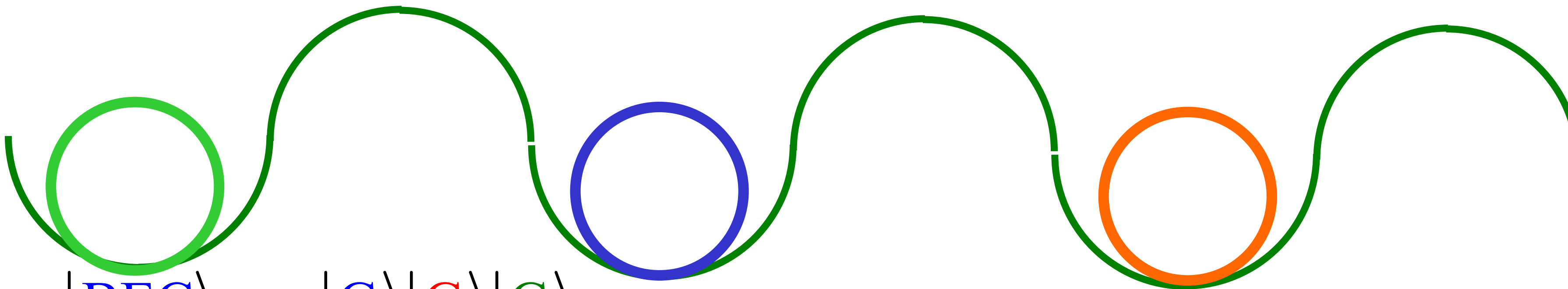

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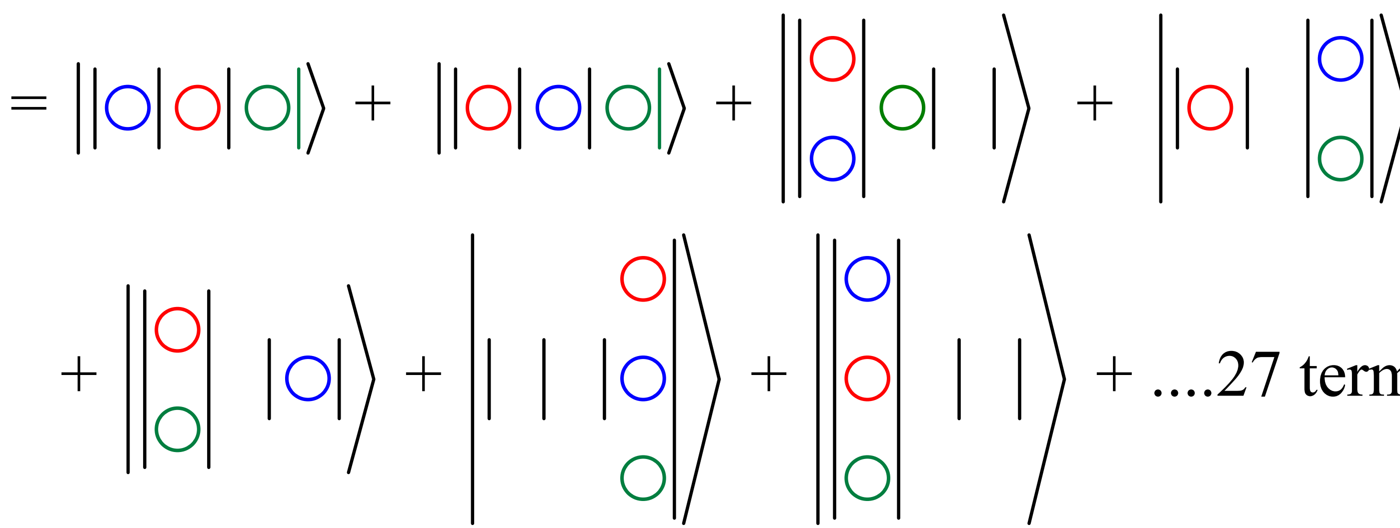

+ ....27 terms

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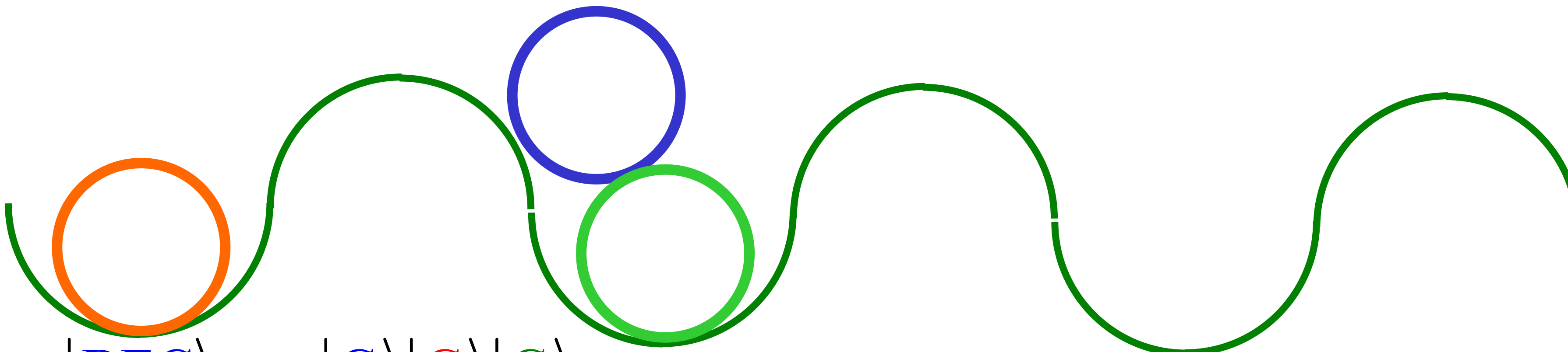

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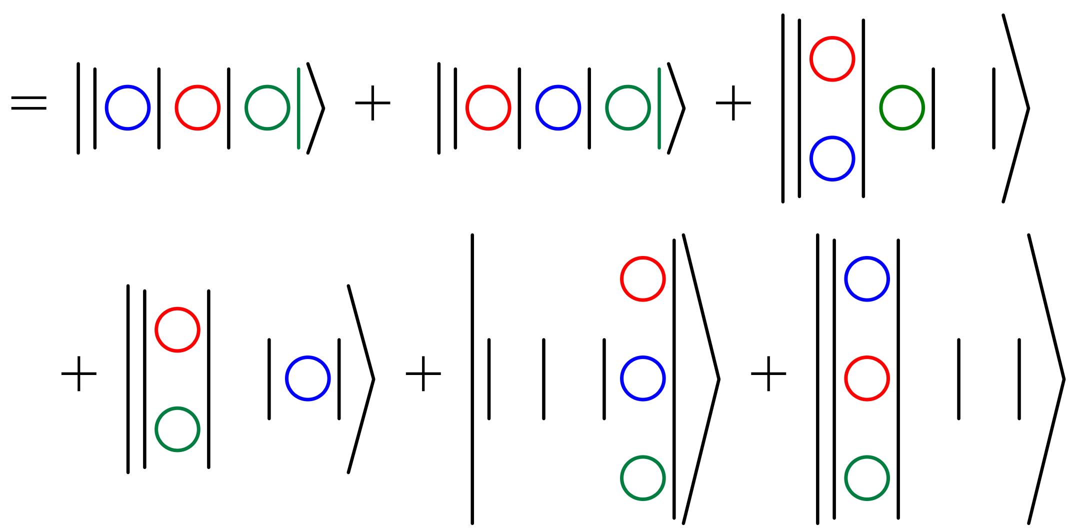

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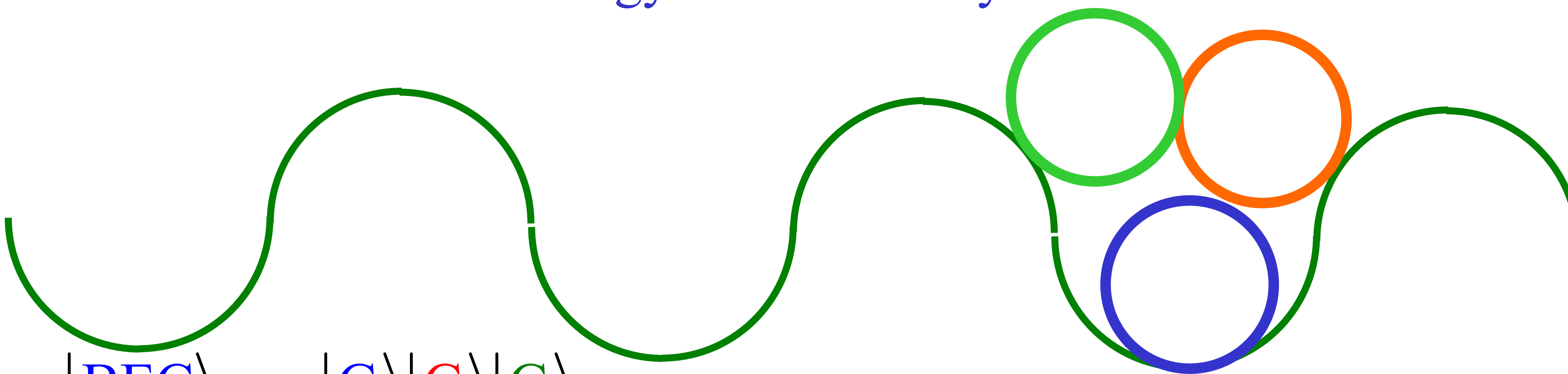

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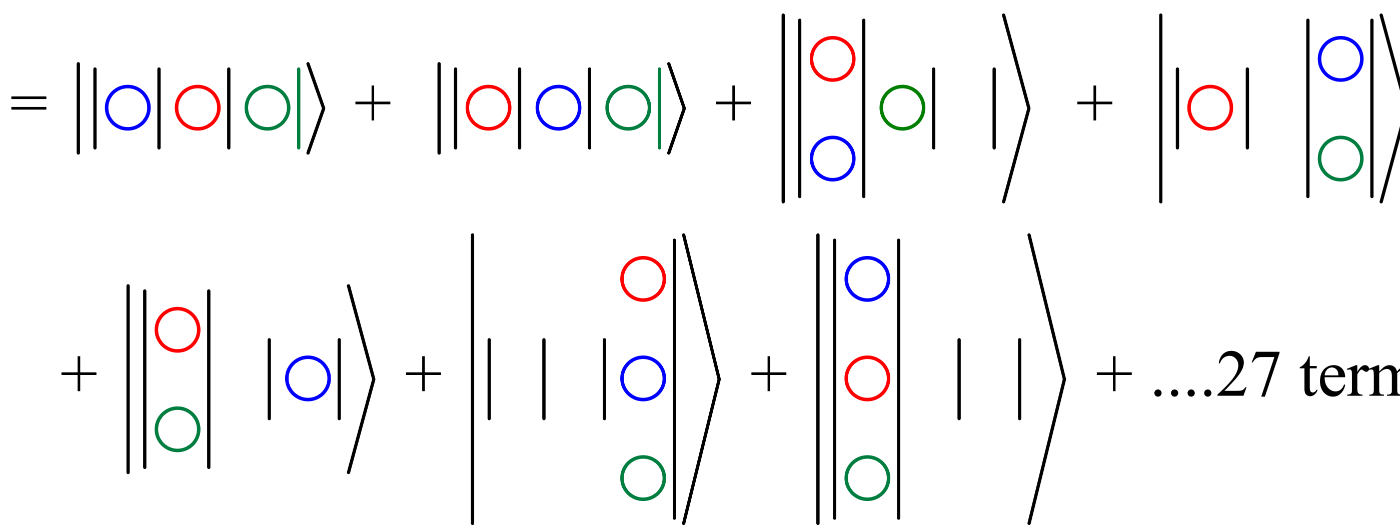

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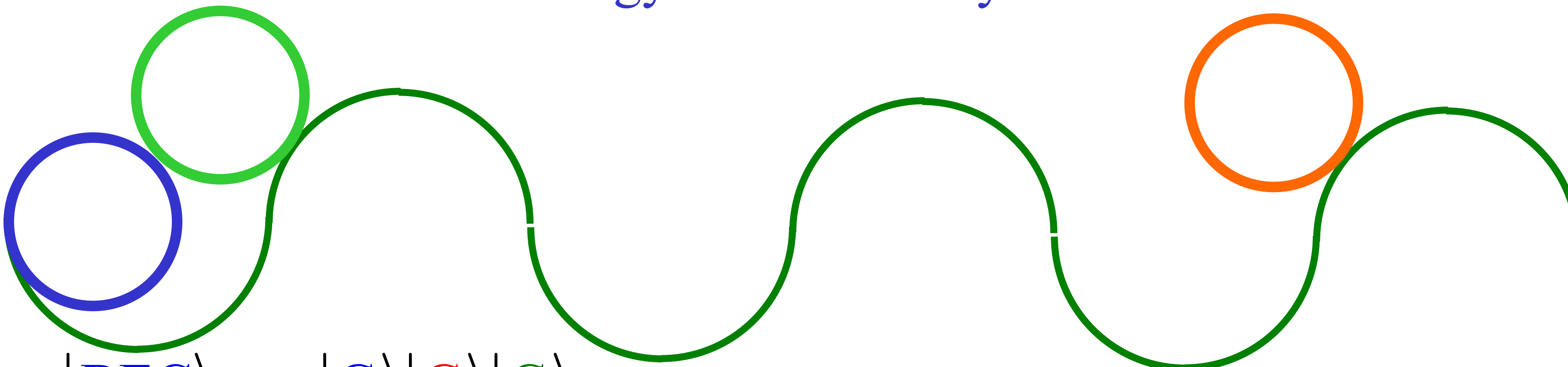

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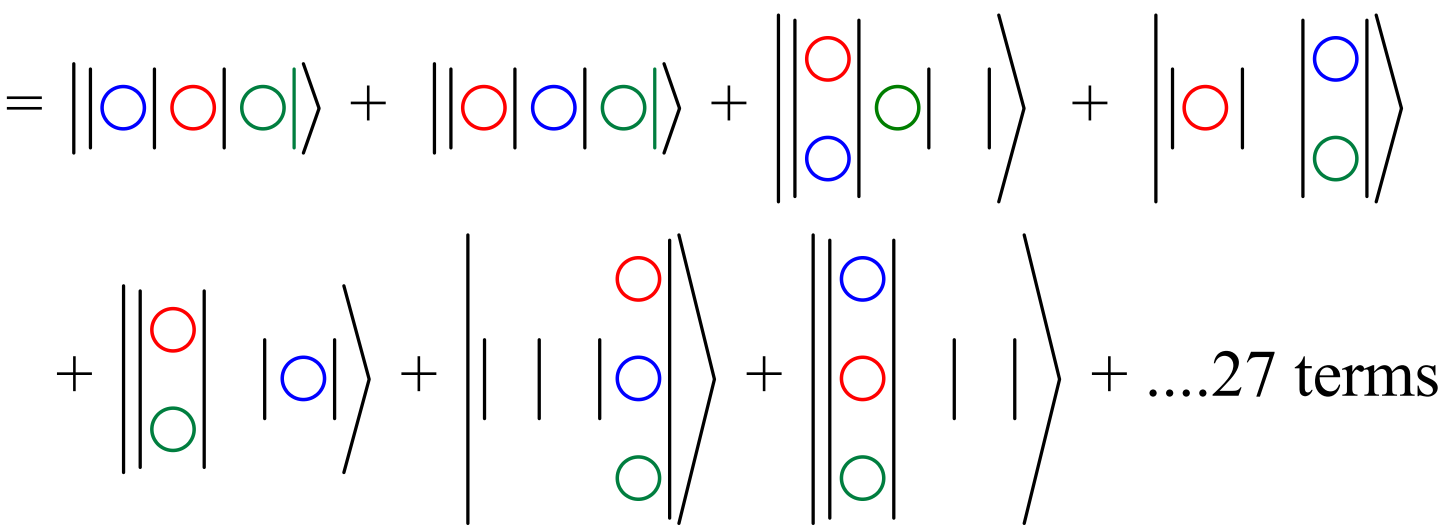

Large fluctuations in number of atoms in each potential well – *superfluidity* (atoms can "flow" without dissipation)

3. Breaking up the Bose-Einstein condensate

By tuning repulsive interactions between the atoms, states with multiple atoms in a potential well can be suppressed. The lowest energy state is then a *Mott insulator* – it has negligible number fluctuations, and atoms cannot "flow"

$$
\begin{aligned}
\left|\mathrm{MI}\right\rangle = & \left|\,|{\color{blue}\bigcirc}|{\color{red}\bigcirc}|{\color{green}\bigcirc}|\right\rangle + \left|\,|{\color{red}\bigcirc}|{\color{blue}\bigcirc}|{\color{green}\bigcirc}|\right\rangle + \left|\,|{\color{blue}\bigcirc}|{\color{green}\bigcirc}|{\color{red}\bigcirc}|\right\rangle \\
& + \left|\,|{\color{green}\bigcirc}|{\color{blue}\bigcirc}|{\color{red}\bigcirc}|\right\rangle + \left|\,|{\color{red}\bigcirc}|{\color{green}\bigcirc}|{\color{blue}\bigcirc}|\right\rangle + \left|\,|{\color{green}\bigcirc}|{\color{red}\bigcirc}|{\color{blue}\bigcirc}|\right\rangle
\end{aligned}
$$

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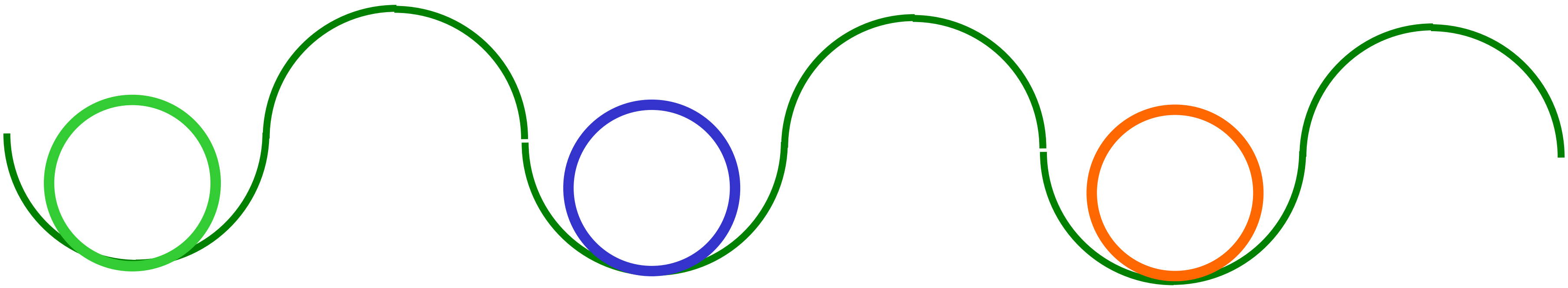

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$$+ \big|\,|{\color{green}\bigcirc}|{\color{blue}\bigcirc}|{\color{red}\bigcirc}|\big\rangle + \big|\,|{\color{red}\bigcirc}|{\color{green}\bigcirc}|{\color{blue}\bigcirc}|\big\rangle + \big|\,|{\color{green}\bigcirc}|{\color{red}\bigcirc}|{\color{blue}\bigcirc}|\big\rangle$$

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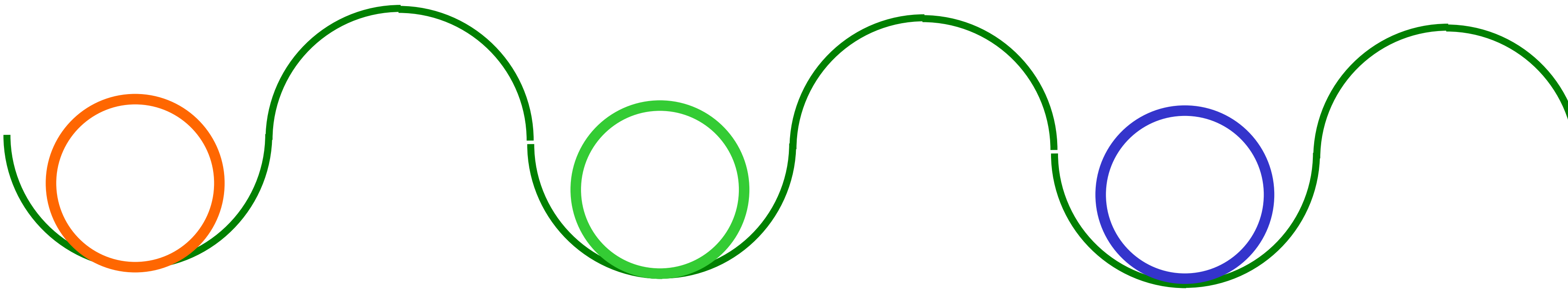

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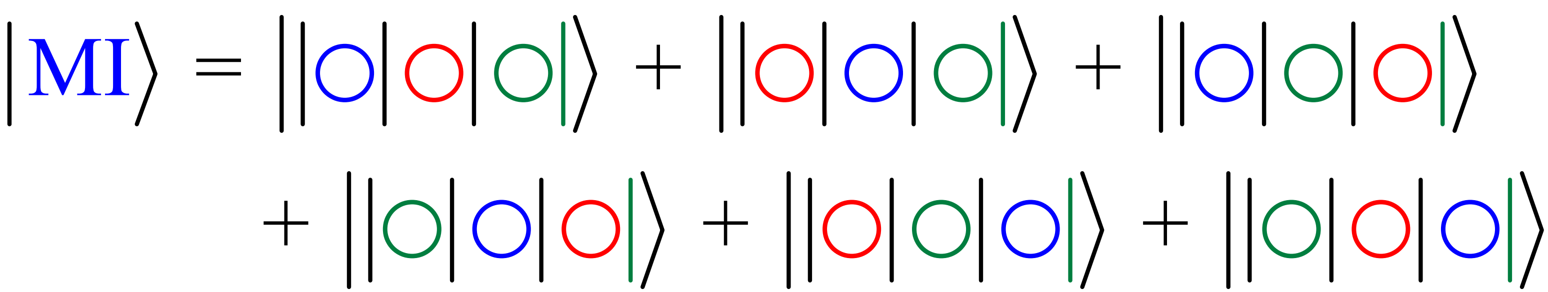

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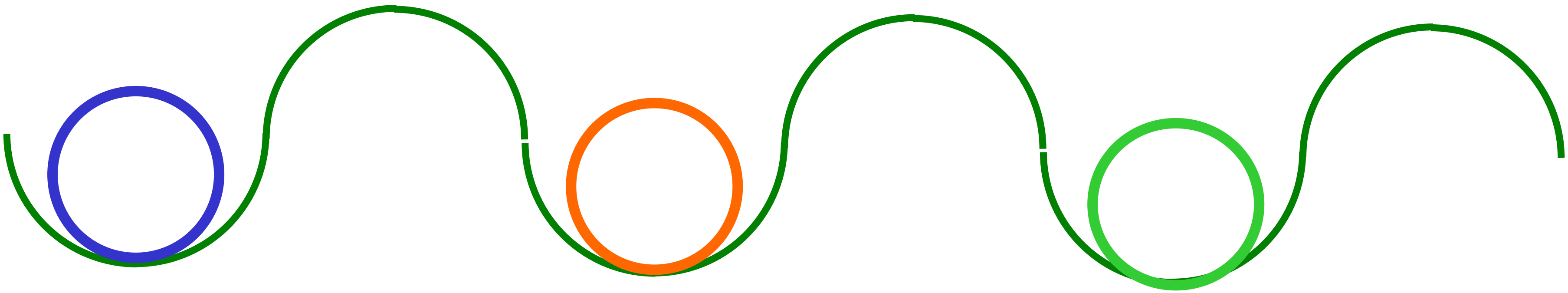

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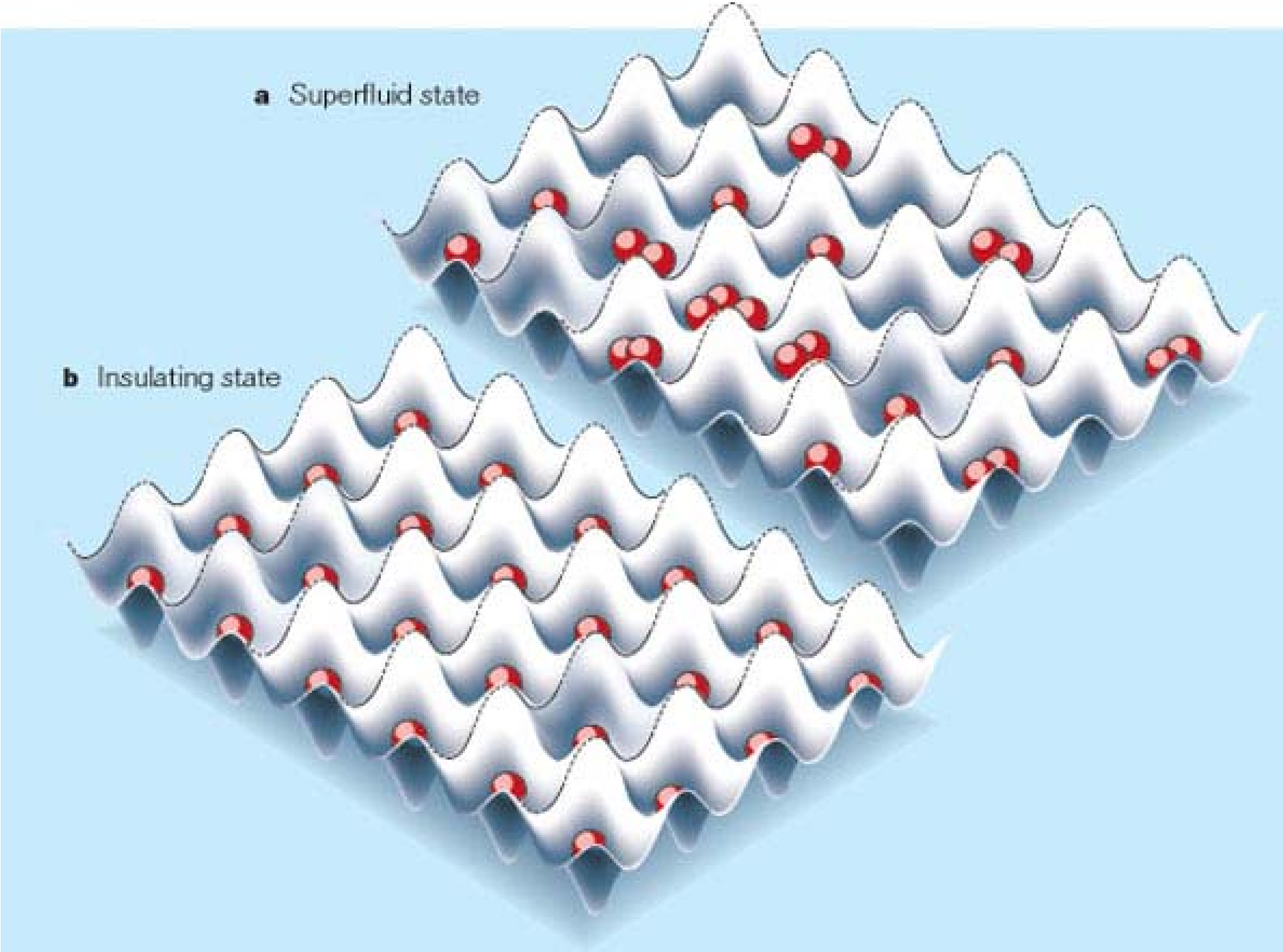
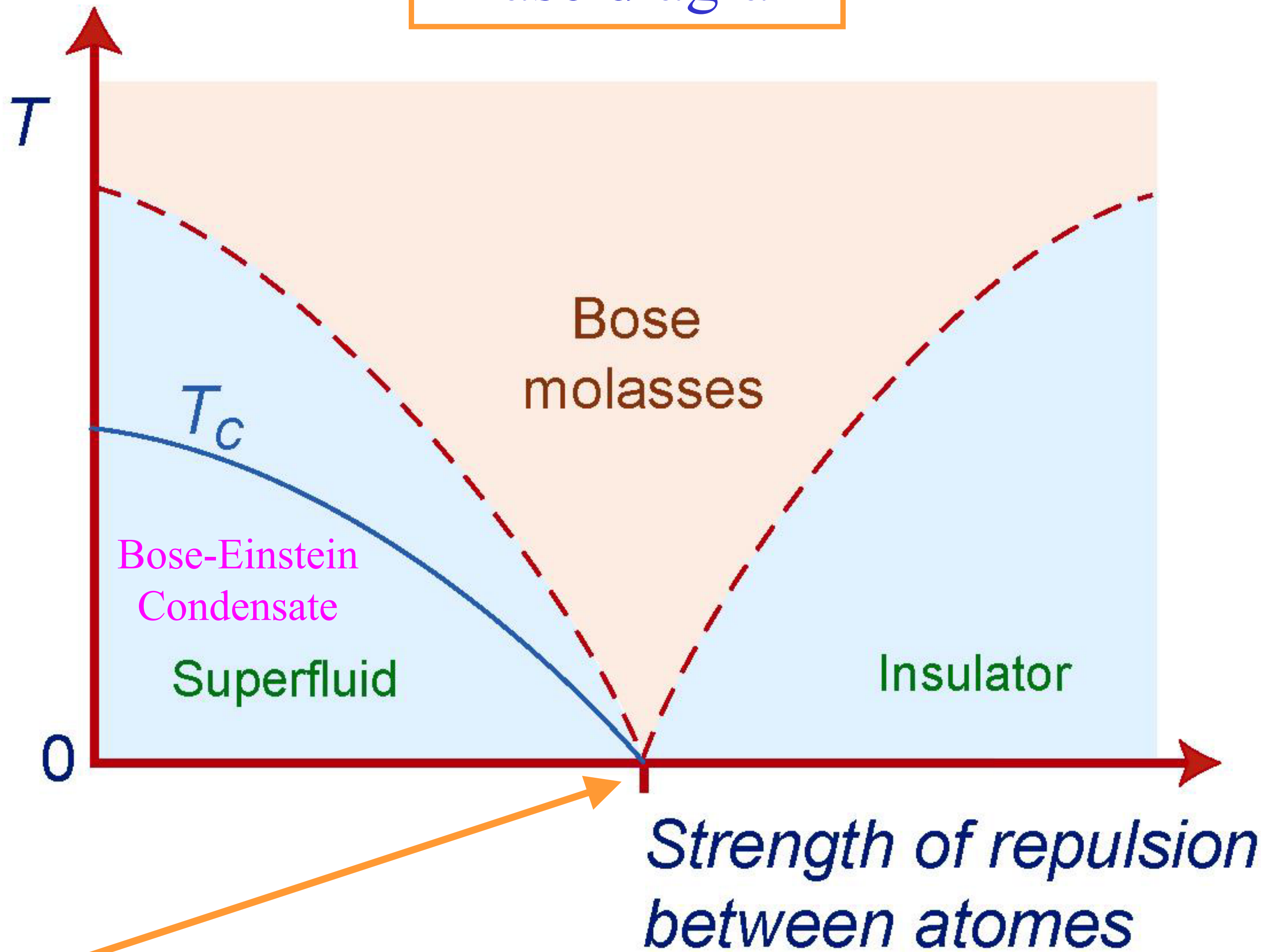
$$+ \left|\,|{\color{green}\bigcirc}|{\color{blue}\bigcirc}|{\color{red}\bigcirc}|\right\rangle + \left|\,|{\color{red}\bigcirc}|{\color{green}\bigcirc}|{\color{blue}\bigcirc}|\right\rangle + \left|\,|{\color{green}\bigcirc}|{\color{red}\bigcirc}|{\color{blue}\bigcirc}|\right\rangle$$


a Superfluid state
b Insulating state

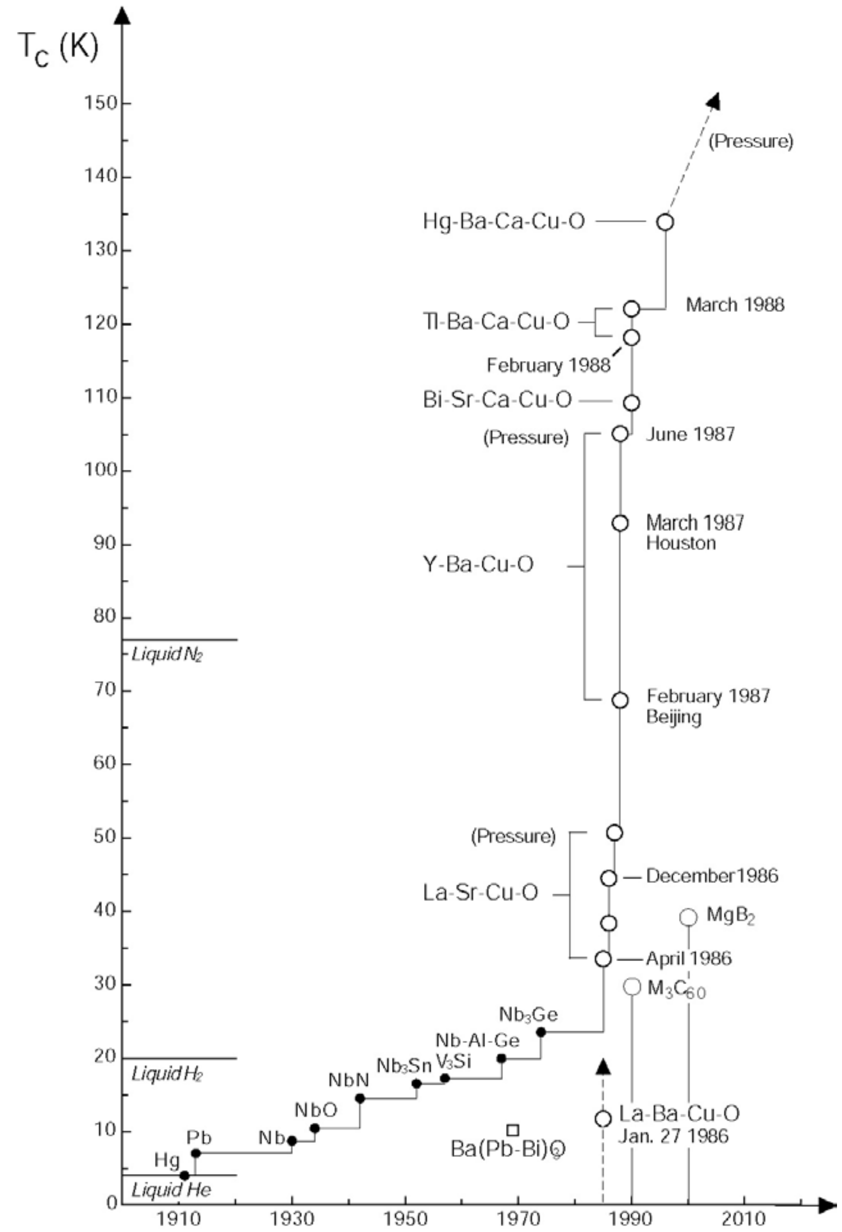
Phase diagram



Quantum phase transition

4. The cuprate superconductors

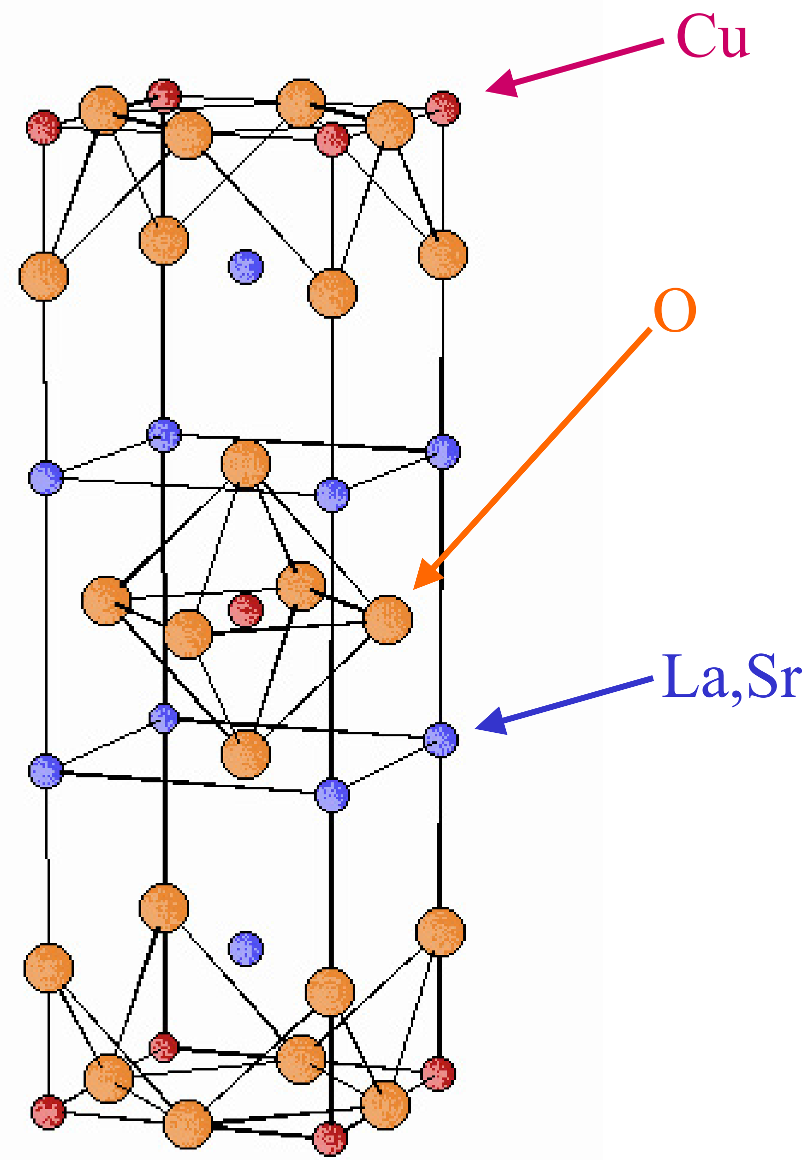
A superconductor conducts electricity without resistance below a critical temperature T_c

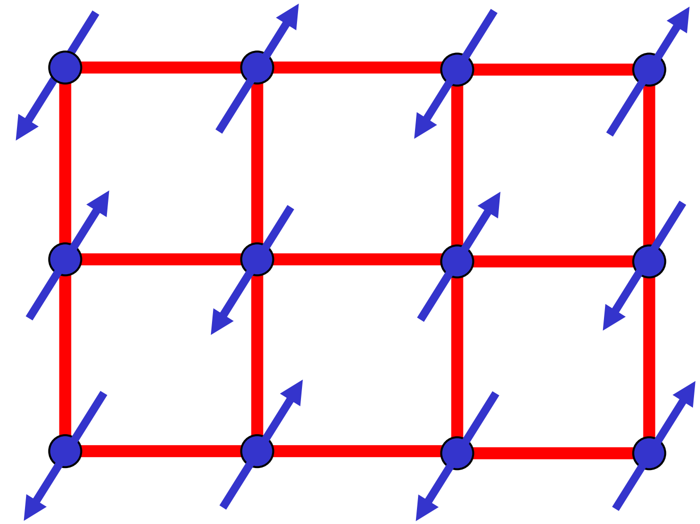


La_2CuO_4 ---- insulator

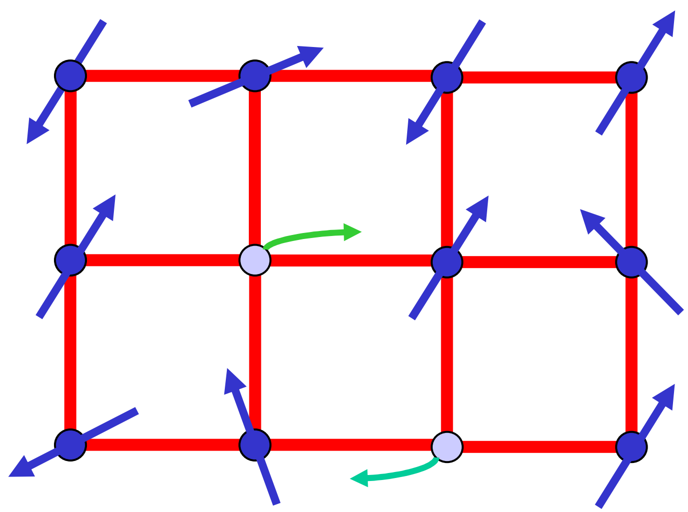
$La_{2-x}Sr_xCuO_4$ ---- superconductor for $0.05 < x < 0.25$

Quantum phase transitions as a function of Sr concentration x



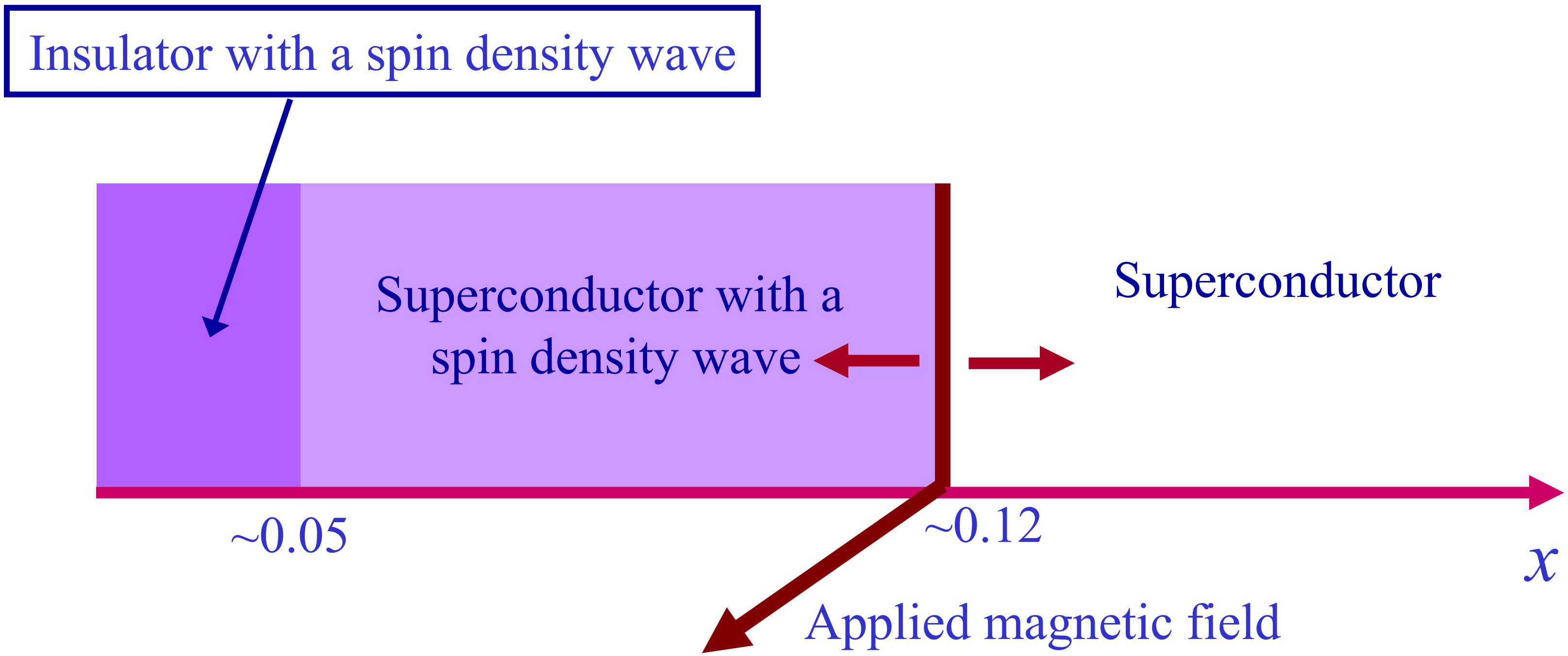


La_2CuO_4 --- an insulating ***antiferromagnet*** **with a *spin density wave***



$La_{2-x}Sr_xCuO_4$ ---- a ***superconductor***

Zero temperature phases of the cuprate superconductors as a function of hole density



Theory for a system with strong interactions: describe superconductor and superconductor+spin density wave phases by expanding in the deviation from the quantum critical point between them.

Accessing quantum phases and phase transitions by varying "Planck's constant" in the laboratory

- ***Immanuel Bloch***: Superfluid-to-insulator transition in trapped atomic gases

- ***Gabriel Aeppli***: Seeing the spins ('qubits') in quantum materials by neutron scattering

- ***Aharon Kapitulnik***: Superconductor and insulators in artificially grown materials

- ***Matthew Fisher***: Exotic phases of quantum matter